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International Workshop
on
MATHEMATICAL METHODS IN COMBUSTION



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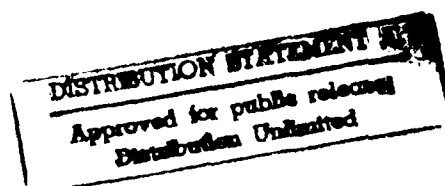
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Centro di Cultura Scientifica "A. Volta"
Villa Olmo, Como, Italy

18-22 May 1992

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Mathematical Methods in Combustion

Monday, 18 May 1992 Villa Olmo, Room "Olimpo"

08.30 Registration

09.15 **L. De Luca, R. Reichenbach, V. Calarese**
Introductory Remarks

ANALYTICAL FUNDAMENTALS

B.V. Novozhilov chairman

09.30 **B.J. Matkowsky**
Synergism of Analytical and Numerical Approaches in Combustion

10.30 **A. Tesei**
Blow-Up of Phenomena for Some Parabolic and Hyperbolic Models in Combustion Theory

11.00 *coffee break*

11.30 **A.G. Merzhanov**
On the Role of Computer-Aided Calculations in Combustion Theory

12.00 **C.D. Pagani, M. Verri, and S. Salsa**
Nonlinear Burning Stability of Solid Propellants: an Analytical Approach

12.30 **B.V. Novozhilov**
On the Theory of Surface Spin Burning

13.00 **R. Dal Passo**
On a Moving Boundary Problem Arising in Fluidized Bed Combustion

13.30 *lunch*

MATHEMATICAL APPLICATIONS

B.J. Matkowsky chairman

14.30 **L. De Luca**
Nonlinear Transient Burning of Solid Propellants: a Simple Example of Synergism between Analytical and Numerical Methods

15.00 **D. Grune and D. Heisel**
Burning Behaviour of Solid Propellants at High Pressure and High Loading Density

15.30 *coffee break*

16.00 **N. Kidin**
Acoustics and Control of Combustion Instabilities

16.30 **F.E.C. Culick**
An Application of Dynamical Systems Theory to Nonlinear Combustion Instabilities

17.00 Round Table Discussion

17.30 End of Session

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Tuesday, 19 May 1992 Villa Olmo, Room "Olimpo"

8.50 **L. De Luca**
Introductory Remarks

NUMERICAL FUNDAMENTALS

A. Quarteroni chairman

- 09.00 **E.S. Oran**
Limitations and Potentials of Numerical Methods for Simulating Combustion
- 10.00 **C. Di Blasi**
Numerical Simulation of the Dynamics of Flame Spreading over Liquid Fuels
- 10.30 **M.Kh. Schur**
Navier-Stokes Simulation of Supersonic Combustion in Continuous Wave HF-Chemical Lasers Based on Compressibility Scaling Method
- 11.00 *coffee break*
- 11.30 **G. Continillo and S. Baruffo**
On the Approximation of Chemical Reaction Terms in Finite-Difference Calculations
- 12.00 **G. De Michele, S. Pasini, and A. Tozzi**
Combustion Optimization in Power Station Boilers by Advanced Modeling Technology
- 12.30 **R. Heiser**
A Navier-Stokes Solution of the Heat Transfer to Gun Barrels
- 13.00 **F. Magugliani**
Computers in Science and Engineering Practical Applications
- 13.30 *lunch*

DETONATION PROCESSES

E.S. Oran chairman

- 14.30 **O. Nekhamkina and M.Kh. Strelets**
Application of Efficient Riemann Solver and TDV Scheme for Numerical Simulation of Detonation Waves in Hydrogen-Oxygen Mixtures
- 15.00 **M. Valorani and M. Di Giacinto**
Numerical Analysis of Detonative Processes
- 15.30 *coffee break*
- 16.00 **H.E. Longtin and P. Clavin**
Critical Conditions for Detonation Initiation by Non Uniform Hot Pockets of Reactive Gases
- 16.30 **A. Lunardi**
Stability of Travelling Waves in Deflagration to Detonation Transition Models
- 17.00 Round Table Discussion: Assessment of Numerical Methods
A. Trovati: Numerical Simulation in Combustion: Industry Needs and Perspectives
- 17.30 End of Session

Wednesday, 20 May 1992 Villa Olmo, Room "Olimpo"

08.50 **L. De Luca**
Introductory Remarks

LINEAR COMBUSTION STABILITY

A.G. Merzhanov chairman

09.00 **B.V. Novozhilov**
Combustion Stability of Solid Propellants ZN- and FM- Approaches

09.30 **P. Clavin**
Acoustic Instabilities of Flames

10.00 **V.E. Zarko and A.B. Kiskin**
Stability and Transient Radiation-Driven Solid Propellant Combustion

10.30 **J. Yin**
Studies on Mathematical Models of Solid Propellant Combustion at Northwestern Polytechnical Institute, Xi'an, China

11.00 *coffee break*

11.30 **M.Q. Brewster and S. Son**
Mathematical Modeling of Unsteady Combustion of Energetic Solids Subject to External Radiation

12.00 **F. Cozzi and L. De Luca**
Radiation-Driven Frequency Response Function by Flame Models

12.30 Round Table Discussion: Linear Combustion Stability

13.30 *lunch*

CLOSURE SESSION

C.D. Pagani chairman

14.30 **R. Reichenbach, D. Mann and V. Calarese**
US Guidelines for Research Proposals

15.00 **P. Clavin, B.J. Matkowsky, B.V. Novozhilov, C.D. Pagani and A. Tesei**
Future Perspectives in Analytical Methods

15.30 *coffee break*

16.00 **E.S. Oran, M.Kh. Strelets, M.Kh. Schur and C. Di Blasi**
Future Perspectives in Numerical Methods

16.30 General Discussion

17.15 **L. De Luca**
Summary and Conclusions

17.30 Closure of Workshop

International Workshop_
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List of abstracts

Centro di Cultura Scientifica "A. Volta"
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18-22 May 1992

Synergism of Analytical and Numerical Approaches in Combustion

B.J. Matkowsky
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and Applied Mathematics
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We employ a synergism between analysis and large scale scientific computations to investigate problems of both solid and gaseous fuel combustion. Since activation energies in combustion problems are generally large, reaction is typically confined to a thin zone. In the asymptotic limit of very large activation energies, the reaction zone shrinks to a moving surface, termed a front, and the problem is reduced to a free boundary problem, in which determination of the front is part of the solution of the problem. Our analytical studies correspond to the case of a front, while our numerical computations correspond to finite, though large, activation energies. Since the solution of the problem exhibits rapid change through the reaction zone, accurate resolution of solution behavior poses a challenge, which is met by an adaptive pseudo-spectral method which we introduce. Our investigations are characterized by the interplay between analysis and numerical computation.

In solid fuel combustion a high temperature thermal wave propagates through a sample, converting reactants to products. In addition to the uniform mode of propagation, in which a planar front moves with constant velocity, other modes of propagation have been observed. These include (i) pulsating combustion - in which the velocity of a planar front oscillates in time, (ii) spinning combustion - in which a hot spot(s) moves in a helical path along the surface of a cylindrical sample, (iii) multiple point combustion - in which the hot spots appear, disappear and then reappear, and (iv) spiral combustion - in which a hot spot moves along a spiral path on a planar sample. We describe these and other combustion modes, including those exhibiting chaotic behavior.

In gaseous fuel combustion in two dimensions, we consider the problem of a flame stabilized on a fuel source. In addition to an axisymmetric flame front, separating burned from unburned gases, we describe various types of flames, including (i) pulsating axisymmetric flames, (ii) stationary cellular flames, (iii) cellular flames with traveling waves, standing waves, quasi-periodic waves and chaotic waves along the front.

Finally, we describe a method which combines our adaptive pseudo-spectral method with domain decomposition ideas, to solve problems with more complex chemical kinetics. Specifically, we illustrate the method for a problem with a sequential reaction mechanism.

**Blow-up of Phenomena for Some Parabolic and Hyperbolic
Models in Combustion Theory**

Alberto Tesei
Dipartimento di Matematica "G. Castelnuovo"
Università di Roma "La Sapienza", Roma, Italy

Even the simplest mathematical models of combustion phenomena are inherently nonlinear. As a consequence, the superposition principle is not valid and novel "dissipative" phenomena arise, due to the mutual interaction between diffusion, convection and bulk heat sources or sinks.

The space-time evolution of such phenomena can be qualitatively studied in detail using simple parabolic or hyperbolic models. A number of methods has been devised for such investigation. We mention in particular the group analysis of nonlinear equations, comparison methods and the construction of stable numerical algorithms for conservation laws.

In this lecture we review some of the above topics, with an emphasis on phenomena of thermal runaway. In this general framework, we shall also present new results concerning blow-up of solutions for quasilinear hyperbolic conservation laws.

**On the Role of Computer-Aided Calculations
in Combustion Theory**

A.G. Merzhanov
Institute of Structural Macrokinetics
Russian Academy of Sciences
142432 Chernogoloka, Moscow Region, Russia

The computer-aided numerical solutions to the equations of thermal conductivity and diffusion with the nonlinear heat and mass sources originating from chemical reactions were first used for obtaining the quantitative results of some specified, particular cases of interest. Then it was understood that a multitude of such calculations, termed the "numerical experiment", could provide a powerful tool for theoretical studies.

Discussed is the role of computer-aided calculations in combustion theory aiming at:

- Obtaining the interpolation formulae that may substitute the explicit solutions.
- Numerical checking the approximate explicit solutions (provided by approximate theories).
- The studies on the mechanism of the processes; elucidating the major and minor factors (terms of equations); preparing the equations for finding the approximate solutions.

Considered is a number of theoretical problems solved by the author and his colleagues at one time by using computers (hot spot thermal explosion, transition from self-inflammation to ignition, combustion in a flow, degeneration of combustion wave, self-ignition of metal particles and suspended drops, auto-oscillating combustion and spinning waves, etc.).

NONLINEAR STABILITY IN SOLID PROPELLANT COMBUSTION:
A THEORETICAL APPROACH

C.D.Pagani, S.Salsa, M.Verri

Dipartimento di Matematica del Politecnico, Milano, Italy

A nonlinear reaction-diffusion equation on a half-line, arising in solid propellant combustion theory, is considered. The propellant is subjected to an external radiant flux; furthermore, it is assumed adiabatic and optically opaque except at the burning surface, where chemical reactions are concentrated. We investigate the existence of uniformly propagating thermal waves and discuss their asymptotic stability. The problem is formulated in an abstract setting as an initial value problem in a suitable Banach space for a fully nonlinear parabolic equation. The obtained stability/instability results are valid for a large class of pyrolysis laws and flame submodels which are incorporated in the governing equation of the system.

ON THEORY OF SURFACE SPIN BURNING

BORIS V. NOVOZHILOV

*Institute of Chemical Physics, Russian Academy of Sciences,
Moscow, 117977, Russia*

The problem of spin combustion is taken as an example to discuss various methods (analytical, numerical and approximate) in combustion theory.

For the first time spin burning has been observed during the burning of porous metallic specimens in gaseous oxidizer. At ignition of the cylinder sample a glowing spot of small diameter appears on its side surface, moves in a spiral along the side surface of an unburnt part of the sample. The sample burns along the side surface; the inner part of the sample either does not burn up at all, or reacts completely after the surface combustion front has passed.

The spin burning problem is liable to analytical solution only in the vicinity of the stability boundary, where the departure of the burning regime from the steady-state is considered to be small. A number of papers were devoted to the theoretical investigation of the problem with the help of bifurcation theory. There are only a few study where a pronounced non-linear regime of spin combustion was treated numerically.

It must be mentioned that the spin burning has been realized both analytically and numerically with very small cylinder diameters. Real experiments are run, as a rule, with specimens of a much larger diameters.

The approximate analytical method is formulated for the surface spin combustion in this paper. It is assumed in a two-dimensional model that the unburned fuel as well as the combustion products are both solid and a condensed phase exothermic reaction occurs on the cylindrical surface, with the combustion centre penetrating into the specimen to a small depth. Because the spin spot motion is almost perpendicular to the vector of the combustion wave mean velocity the two-dimensional problem can be reduced to a simple one-dimensional one, which is similar to the problem of combustion with heat losses.

The conditions of existence of spin regime are obtained. Explicit analytical expression for various quantities of interest, including the propagation spin velocity, the wave mean velocity and the temperature profile are given. They depend on the cylinder diameter and heat losses. As the diameter grows two or more centres of the chemical reaction appear (multi-centre spin) on the cylinder surface.

Wherever possible, conclusions of the above mentioned approaches are compared with the experimental data and the numerical results.

On a Moving Boundary Problem Arising
in Fluidized Bed Combustion

R. Dal Passo
Istituto per le Applicazioni del Calcolo "M. Picone"
Consiglio Nazionale delle Ricerche Roma, Italy

We consider a model describing the combustion of a coal particle in a fluidized bed, in which attrition plays a dominant role. The model consists of: 1) a quasilinear elliptic equation for the oxygen concentration, supplemented by boundary conditions on the moving surface representing the burning particle interface; 2) an ordinary evolution equation for the carbon consumption; 3) an equation governing the motion of the interface in terms of a specified function of the carbon consumption at the interface. We prove a global existence and uniqueness result, together with a-priori bounds for the solution; the existence of travelling waves will also be established.

**NONLINEAR TRANSIENT BURNING OF SOLID PROPELLANTS:
A SIMPLE EXAMPLE OF SYNERGISM
BETWEEN ANALYTICAL AND NUMERICAL METHODS**

Luigi De Luca

*Dipartimento di Energetica, Politecnico di Milano
32 Piazza Leonardo da Vinci, 20133 Milano, Italy*

ABSTRACT

A comprehensive nonsteady combustion model, capable of computing transient burning rates and predicting intrinsic combustion stability of solid rocket propellants, is described based on quasi-steady thermal flames. This overall model includes several appropriate submodels. The transient flame submodel is capable of describing spatially thick gas-phase flames, by accommodating any flame thickness and allowing pressure and/or temperature dependence of several of the relevant parameters. The transient condensed-phase submodel accounts for temperature dependent properties and possible volumetric processes (distributed chemical reactions and/or in-depth absorption of radiation emitted by an external source). The pyrolysis submodel pictures irreversible processes concentrated at the burning surface and/or volumetrically distributed. Within current limitations, the resulting overall transient combustion model is widely applicable, but fundamental work in the area of high temperature chemical kinetics, characteristic gas-phase times, condensed-phase heterogeneity, and surface processes is badly needed.

The overall model can either be solved numerically to follow burning histories or analyzed on the basis of stability theories to predict final burning outcomes. This allows a convenient synergism between analytical and numerical methods, shedding much needed light if properly carried out. Intrinsic combustion stability properties are analyzed from both a linearized and a nonlinear but approximate viewpoints. In the former case, attention is focused on sinusoidal frequency response function. In the latter case, both static and dynamic (or transitional) stability features are discussed by introducing a nonlinear algebraic static restoring function. Dynamic extinction vs static extinction is clarified; deflagration limits are deduced for pressure and other parameters as well; effects of combustion diabaticity are examined; connections with the Zeldovich-Novozhilov approach are briefly discussed. Bifurcation plots are obtained suggesting, for the steady-state solution, a possible transition from time-invariant to oscillatory self-sustained for most of the combustion parameters; these analytical expectations are numerically verified. All results, whether obtained under linear or nonlinear conditions, may markedly depend on the enforced transient flame submodel.

**Burning Behavior of Solid Propellants at High Pressure
and High Loading Density**

D. Grune and D. Hensel
French-German Research Institute of Saint Louis (ISL)
Saint Louis, France

The burning behavior of colloid propellants is briefly described by the VIEILLE's law of burning, which applies to the range of pressure involved in weapons. For single-base, double-base, and heterogeneous propellants it will be shown by means of closed vessel tests that the VIEILLE's law is not applicable to the complete pressure range. Therefore, the spatial law of burning is modified by means of an empirically perturbing term to describe the combustion of the foregoing propellants as a function of both pressure and porosity of the propellant bed. To study the parameters of this novel spatial law, the pressure history in the closed vessel test is simulated with the interior ballistic code AMI - a two dimensional two-phase model - by varying the different parameters, until an approximate agreement between numerical and experimental investigation is reached.

Limitations and Potentials of Numerical Methods for Simulating Combustion

Elaine S. Oran
Laboratory for Computational Physics and Fluid Dynamics
Naval Research Laboratory
Washington, DC 20375

The capability of numerical simulations to describe combustion processes and systems will always be limited by

- Computer speed and memory available. For simulating combustion, we need to resolve extremely disparate time and space scales. Further, we will always want to resolve more and more scales and contributing phenomena, and therefore better describe the system.
- Efficiency of our algorithms and their implementation. Algorithms that make the best use of computer resources usually imply some trade-off between accuracy and efficiency. The important point is to choose algorithms that are accurate *enough* and most efficient.
- Availability of adequate input data. This refers to information such as participating chemical species, chemical reaction rates, thermodynamic properties, and radiation intensities.

This presentation addresses the first two issues, computers and algorithms, and considers the limits of what we are able to simulate. We have learned that the way to stretch this limit is to break the full problem into a number of submodels, each representing a contributing physical process such as convection or conduction, solve for the effects of each process with an accurate enough algorithm optimized for the particular computer, and then combine these results. Recently, we have had access to massively parallel computers in which many computer processors carry out simultaneous mathematical operations and then this information is coordinated. Such computers present the possibility of performing computations an order of magnitude or more faster than conventional computers. Here we describe numerical simulations of several types of combustion problems, ranging from laminar and diffusion flames to turbulent reacting flows, and use these as vehicles for explaining the trade-offs in accuracy, efficiency, and implementation on parallel computers.

NUMERICAL SIMULATION OF THE DYNAMICS OF FLAME SPREADING OVER LIQUID FUELS

C. Di Blasi

*Dipartimento di Ingegneria Chimica, Università di Napoli
Piazzale V. Tecchio, 80125 NAPOLI, Italy*

An unsteady, two-dimensional mathematical model, including finite rate combustion kinetics, buoyancy effects and transport phenomena for both the gas and the liquid phase, has been numerically solved to simulate flame spread over liquid fuels. The vaporization process is described through empirical expressions relating the vapor pressure to surface temperature while the effects due to surface tension variation are properly accounted for by means of the boundary conditions for momentum equations at the liquid/gas interface.

In agreement with experiments, the flame propagates steadily even for initial liquid temperatures below the flash point. Moreover, as the initial liquid temperature is further decreased, the propagation occurs according to a pulsating behaviour and, for very low temperatures, with a uniform rate again. Numerical simulations have shown that oscillatory phenomena of flame spread are always associated with the presence of surface tension driven motions in the liquid phase. The presence of the flame above a liquid, below the flash point, causes a non-uniform temperature distribution. Given the dependence of surface tension on temperature, a gradient in the surface tension is also established, which drives motions from the warm region under the flame to the cool region ahead of the flame. Thus an eddy is formed in the liquid phase, ahead of the flame, which represents an important mechanism for the pre-heating of the liquid to the flash point. Under normal gravity conditions, liquid phase buoyancy does not seem to affect the flame spread process. On the contrary, gas phase buoyancy, because of the higher temperatures due to combustion processes, plays a primary role and induces a convective flow field which opposes the spread of the flame. As a consequence of surface tension driven flows and of the shear at the liquid/gas interface, a circulating eddy is also formed in the gas phase ahead of the flame.

Gas and liquid phase convective heat transfer makes the surface temperature to increase in a narrow region ahead of the flame, up to give a mixture within the flammability limits. The concurrent gas phase velocities at the flame leading edge and the pre-mixed flammable region over the liquid surface allows the flame to accelerate. Once this high surface temperature region has been passed across, the flame decelerates because the liquid, immediately ahead of the flame, is again below the flash point. Oscillations in the flame spread rate are associated with oscillating values of the intensity of the surface tension driven flow. Surface velocities increase with surface temperature gradients which are alternatively large, when no pre-mixed region exists ahead of the flame, and small, when the liquid ahead of the flame has been pre-heated to the flash point. Therefore, the formation and the consumption of the pre-mixed flammable mixture ahead of the flame determine the conditions for pulsating spread.

NAVIER-STOKES SIMULATION OF SUPERSONIC COMBUSTION IN CONTINUOUS WAVE
HF-CHEMICAL LASERS BASED ON COMPRESSIBILITY SCALING METHOD

M. Shur

Senior Research Scientist, State Institute of Applied Chemistry,
Dobrolyubov Ave. 14, St.-Petersburg 197198, Russia

Common approach to the numerical simulation of the supersonic continuous wave (CW) chemical lasers is based on successive computation of the nozzle array and laser cavity flows, i.e. on the use of the flow parameter values at the nozzles exit plane, obtained by an independent calculation of fuel and oxidant nozzle flows, as the boundary conditions for the cavity flow computation. Such approach apparently does not permit to describe the upwind influence of the cavity processes on the nozzle flow, which in reality may be of great significance. In particular, without taking this influence into consideration it is impossible to describe adequately the processes in the recirculation zone behind the nozzle array base, which affect strongly the evolution of mixing layers and combustion in the cavity, and consequently control the laser efficiency. Moreover, the regimes of laser operating may exist, when the great difference of the nozzle exit pressures causes the boundary layer separation inside the nozzle array. In such a situation the combustion may start directly in the nozzles because of diffusion of reactants into the separation region. The only way one could describe all these phenomena is the coupled Navier-Stokes simulation of the flow in the domain of complex geometry, which contains, along with the cavity region, at least the supersonic parts of the fuel and oxidant nozzles.

In the present work for this purpose a new Navier-Stokes code is created, which is based on recently developed Compressibility Scaling Method (CSM). The most important feature of this method is insensitivity of its convergence rate to the flow Mach number Mo , including arbitrary small values of the parameter. Due to this fact, when computing the flows under consideration (mixed subsonic and supersonic flows with large zones of recirculation and/or low Mach numbers), CSM has significant advantages over traditional implicit methods for the compressible Navier-Stokes equations, which efficiency decreases sharply at low Mo values. When simulating the combustion and nonequilibrium processes in the HF chemical laser cavities CSM is coupled with time-saving (without matrix inversions) numerical algorithm of calculation of multicomponent diffusive mass fluxes and with an efficient fully implicit method of computation of the radiation generated by the laser. Capabilities of proposed approach are illustrated by examples of its application for the simulation of the flowfields, combustion, vibrational relaxation and radiative transfer in HF CW chemical lasers with three different designs of nozzle array. Kinetic model of the hydrogen-fluorine combustion, used in computations, included totally 165 elementary reactions between 13 species (H , H_2 , F , F_2 , He , DF , $HF(v)$, $v=0-6$ - vibrational level of the HF molecule). The results presented demonstrate both the efficiency of the code (it provides 3-5 times saving of the computer time over traditional algorithms) and its ability to predict complicated (with shock waves, recirculating zones and mixing/reacting layers) flow pattern. The last claim is supported by good correspondence of numerical and experimental data on flame structure in laser cavity and integral laser output characteristics which cannot be achieved, even qualitatively, by the common approach (successive computation of the nozzle and cavity flows).

On the approximation of chemical reaction terms
in finite-difference calculations

G. Continillo and S. Barruffo

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A popular semi-implicit scheme, widely used as an alternative to the more expensive fully-implicit formulation, is considered. The scheme is roughly equivalent to a pure explicit scheme in terms of computation requirements, is unconditionally stable and has the desirable feature of yielding non-negative values for species concentrations. However, the scheme introduces an error resulting in chemically-inconsistent results, that are not easily recognizable as such. These and more properties of the scheme are illustrated and discussed, and ways of overcoming problems are indicated in the present communication.

HEAT TRANSFER AND COMBUSTION OPTIMIZATION BY ADVANCED MODELING TECHNOLOGY

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ABSTRACT

The problems connected with the limitation of energy resources, with the diversification of fuels and with increasing concern about the effect of emissions on the environment have drawn combustion engineers' attention to the importance of improving combustion equipment design. At the same time, with computational abilities increasing each year, the capability of obtaining detailed information about the combustion process, which involves complex interactions between the fluid dynamics, heat transfer and chemistry, is becoming a reality.

Reviewing the available literature (Richter, 1985, Robinson, 1985, Troe, 1988, Bilger, 1980) we realize that the simultaneous solution of fluid flow, heat transfer and complex kinetics is not yet sufficiently advanced to be applied to real boiler geometries. The aim of the present research is to try to develop a model capable of coupling the fully 3-D solution of fluid flow, heat transfer and complex chemical kinetics (regardless of the kinetic scheme adopted). In this paper attention will be focused mainly on the new algorithm for the solution of the kinetic equations and their coupling with the conservation equation of the time-averaged species.

The combustion model adopted is based on a "quasi-global" scheme, made up of a fuel demolition reaction to CO and H₂ and of a kinetic scheme for transformation to CO₂ and H₂O. The assumption of "fast kinetics", generally utilized in the literature for heat release calculations (e.g. Boyd, 1985, Carvalho 1987) cannot be used in this case, because it permits us only to calculate the final products of the combustion reaction (CO₂, H₂O), and not the intermediate species, that can strongly influence NO formation.

For fuel oil the demolition reaction to CO and H₂ is assumed to have infinite velocity. For methane it is considered with finite velocity K_F , as suggested by Malloggi (1990). The kinetic scheme for the CO/H₂ system was written considering the most important reactions and taking H, O, OH as the radical species. Twenty-five reactions are utilized in the present case, but the program is written in a general form, therefore the kinetic scheme can be easily changed, allowing the testing of different hypotheses.

The species transport equations, after a preliminary transformation are linearized giving a system of N equations in N unknowns that are solved for any cell and for any time step. This algorithm is very suitable for the application to a vectorial machine, and the solution implicitly satisfies mass conservation, element conservation and stoichiometric relations with the maximum precision obtainable with the hardware utilized, as characteristics of solutions in .

As an example of application of the code, results are presented of the simulation of heat transfer, combustion and pollutant formation in a 30 MWt tangentially-fired boiler simulation facility where very detailed in furnace measurements of temperature and main chemical species were taken both in standard and staged combustion conditions. Others applications of the code are described, like design and optimization of a complex combustion system for the application of the reburning process to a 160 MWe power station boiler.

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A Navier-Stokes Solution of the Heat Transfer to Gun Barrels

R. Heiser

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The erosion of gun barrels depends on several influences. As we know temperature is one of the important quantities. Erosion starts at the surface contacting the hot propellant gas. Till now there exists an uncertainty on the real surface temperature or, in other words, do the experiments give the real surface temperature.

The approach of the heat transfer problem reported here tries to stay in the physics of the event as much as possible. The heat transport from the hot propellant gas to the gun barrel is computed by solving the full Navier-Stokes equations for the axisymmetric in-bore flow. This method couples the center-core flow, the boundary layer, the heat transfer, and the heat conduction in the tube wall. Since the boundary layer is considered the steep temperature gradients very close to the bore surface are available. Therefore, the heat flux into the wall is known precisely. The numerical solution is based on an ADI scheme similar to that of Briley-McDonald. A one-equation turbulence model completes the set of equations. Comparison with temperature measurement shows good agreement. The computational method also allows to include coated wall surfaces.

APPLICATION OF EFFICIENT RIEMANN SOLVER AND TVD SCHEME
FOR NUMERICAL SIMULATION OF DETONATION WAVES
IN HYDROGEN-OXYGEN MIXTURES

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The up-to-date nonlinear high order TVD shock capturing schemes provide an efficient tool for the simulation of the ideal gas flows with complicated shock-wave structure. They permit not only to ensure the high accuracy of the numerical solution in the regions of its smooth behavior but also to resolve the shock waves and other modes of discontinuities without flow property spurious oscillations. These features of the TVD schemes can be hardly overestimated and make them very attractive for the numerical simulation of the gas-phase detonation. However some non-trivial problems emerge when extending the TVD schemes, proposed for the calculation of the flows of thermally and calorically perfect gases, to the general case of nonequilibrium reactive flows of the real gas mixtures. One of such problems is connected with the development of the appropriate methods for averaging of the flux Jacobian matrices, which are needed for the approximate Riemann solvers being an important element of the TVD schemes based on the flux-difference-splitting approach. The methods of averaging proposed by now are rather time consuming and besides utilize some a priori non-obvious assumptions, which may lead to decreasing of the accuracy of the numerical solution. In the present work a new method of averaging is developed and embedded into well known Roe's approximate Riemann solver. It is quite simple, provides exact satisfying of the U-property, formulated by P.Roe, can be easily incorporated into any TVD scheme, and applicable for the general case of multicomponent nonequilibrium (finite-rate chemically reacting) mixtures of thermally perfect gases with arbitrary temperature dependence of species internal energies and specific heat capacities. The above properties of the proposed approach, coupled with high order TVD scheme by S.R.Chakravarthy, are illustrated by the two examples of its application for the numerical simulation of detonation waves. The first example deals with the oblique standing detonation wave holding by the wedge in the supersonic flow of the stoichiometric hydrogen-oxygen mixture diluted by argon, and the second one - with the evolution of the detonation induced by the local impulsive energy addition in the enclosure filled with the same mixture. In both cases the same kinetic model of the finite rate hydrogen-oxygen combustion is used, which includes 9 elementary reactions between 6 species (H , O , OH , H_2O , H_2 , O_2).

Numerical Analysis of Detonative Processes

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Numerical simulation of high speed reactive flows must face the challenges prompted by the large differences which may arise between the fluid dynamic time scales, τ_f , and those of the nonequilibrium phenomena, τ_c . A measure of the relative magnitude of these scales is provided by the Damköhler number ($Da = \tau_f/\tau_c$), which has a direct influence on the thickness of the nonequilibrium layers. In the limiting regimes of nearly frozen ($Da \rightarrow 0$) or nearly equilibrium flow ($Da \rightarrow \infty$), there may exist regions in the flow domain, such as solid boundaries or shock waves, where very thin relaxation or chemical layers develop. An insufficient numerical resolution of these layers, by reducing the accuracy and the stability limits of the calculation, may affect the whole flowfield by altering the propagation speed of shocks together with the structure of the nonequilibrium layers at the solid boundaries.

With the proposed numerical model the correct propagation shock speed in reacting gases is achieved by explicitly tracking the shocks and then by integrating the field equations in quasilinear form [1,2]. The stability properties of the scheme are enhanced by a *semi-implicit treatment* of the stiff source terms. The proper level of resolution at the nonequilibrium layers is provided by means of an Adaptive Mesh Refinement (AMR) technique [2].

The motivations backing the choice of a tracking technique are briefly summarized in the following.

The great majority of papers dealing with the numerical simulation of compressible reacting flows have adopted conservative schemes developed in the context of inert gasdynamics. However, there seems to exist some evidence [4,5,6] that when in the nonhomogeneous system of equations the reactive source terms become stiff, one of the most appealing properties of the weak numerical solutions may be lost: the ability of providing the correct propagation speeds of the shocks. The origin of this failure is related to the unavoidable presence of unphysical states, introduced by the shock capturing methods in order to describe the propagation of shocks, which can erroneously trigger the stiff source terms. In order to "deactivate" these states some kind of tracking seems to become necessary for shock capturing methods as well.

Thus, we have deemed proper to follow a classical "fitting" procedure [7] in order to assess its merits and limits in the context of reactive flows. Among the merits it is immediately possible to enlist the following. The enforcement of jump relations across the fitted shocks, if interpreted as a subscale model filtering out the relaxation of chemical processes which evolve on the shortest scales inside the shock transition, can provide an accurate tool to further reduce the overall degree of stiffness displayed by the flow. For example, the "fitting" offers a consistent way of computing the jump relations according to the "partially dispersed" shock model [8] for which the chemistry is frozen across the shock, and vibration is, as the thermodynamic conditions would suggest, alternatively either frozen or in equilibrium.

On the other hand, the issue of an efficient achievement of suitable resolutions at the nonequilibrium layers has been pursued by means of an AMR technique presented in [2]. This technique belongs to the class of embedded, structured grids and it has been designed especially to obtain time accurate solutions.

The generation of the embedded subgrids is performed, independently of the refinement criteria, once and for all at the beginning of the calculation according to a completely recursive algorithm. The tree of subgrids recursively generated takes its root in a relatively coarse, structured, uniform, orthogonal grid containing a number, N_{cell} , of cells which is a multiple of an integer power of two. This root grid is partitioned into an even number of equally sized grids, N_{part} , preset by the user. When any refinement

criterion detects the need of an increased resolution for a cell belonging to one of the parts of the root grid, all cells of this part have their size halved, originating in this way a new subgrid with twice the resolution of the root grid. This procedure holds for all the subgrids of the tree. Therefore, once the pair (N_{cell}, N_{part}) is given, the geometry and the size of all subgrids is uniquely determined, independently of the refinement criterion and of the solution evolution. The refinement criterion "simply" acts as a mean to activate or deactivate the integration over the already generated subgrids.

The time discretization and the order of integration are defined following the asymptotic idea of keeping the solution frozen on the coarser subgrids while letting it evolve on the finer ones. The use of structured grids, together with increasing the grid resolution by consecutive halvings only, reduces to the minimum the number of interpolations required to let the grids follow the propagating signals, and allow an easier coordination of the truncation errors among grids of different resolutions. Both effects improve the space time accuracy of the calculation.

The space-time link between adjacent subgrids is realized by adding extra computational points inside the (hyperbolic) domain of dependence at both sides of each subgrid. These extra points allow the definition of a purely initial value problem for each subgrid, which can thus be solved "independently" from the integration on the other subgrids. This circumstance could become useful in the context of parallel computing.

Once the accuracy requirements have been satisfied by the AMR strategy, then the degree of gasdynamic/chemical stiffness in terms of local Damköhler number is actually reduced or even eliminated. At this point, without problems of stiffness, a fully coupled approach for the solution of the system of equations may become feasible and perhaps even more advantageous than others based on operator splitting. In fact, the fully coupled nonlinear system can be solved very efficiently taking full advantage of the high convergence rate of Newton-type methods.

To summarize, in this work the numerical integration of reactive flows is carried out, over an adaptive computational domain, on the basis of a fully-coupled, quasi-linear formulation of the unsteady, reactive Euler equations. The numerical method presented is obtained by generalizing the second-order λ scheme [7] with explicit "fitting" of shocks to the case of reactive flows.

Results will be presented, in the 1D case, for H_2/O_2 combustion. A detailed chemical kinetics mechanism is adopted. Preliminary tests [3], conducted with more or less tight refinement criteria, show that the use of the proposed AMR technique, in the context hereabove specified, requires a computational work which can be 6-10% smaller than that needed by a uniform grid of the same resolution. Similar savings can be obtained in terms of CPU time. Tables (1) and (2) refers to the following data.

Data for a Uniform Grid

Number of intervals : 2048

Typical number of iterations : 4000

Typical work (number of operations) : $2 \times 2048 \times 4000 = 16,384,000$ (for a two level scheme)

Typical CPU time : 48 hours of IBM RISC 6000/550

Data for the AMR

Base grid resolution : 128 intervals

Number of partitions : 4

Finest level of resolution available : equivalent to a uniform grid of 2048 intervals

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Table 1. Total work		
Test Case	AMR work	% Work
Medium band criterium	885,421	5.4%
Wide band criterium	1,526,694	9.3%

Table 2. Total CPU time		
Test Case	AMR CPU time	% CPU
Medium band criterium	180'	6.2%
Wide band criterium	309'	10.7%

Stability of travelling waves in deflagration to detonation transition models

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We present here some results about the behavior near travelling wave solutions of a class of free boundary parabolic problems with interface conditions. Such problems arise as specific models in one-dimensional combustion phenomena.

Our method can be applied to a number of equations and systems, such as the deflagration-detonation transition model, introduced by J. Ludford and his collaborators:

$$\begin{cases} u_t = u_\eta + u_{\eta\eta}, & \eta \in \mathbf{R}, \eta \neq \xi(t) \\ u(\xi(t), t) = u_*, & [u_\eta]_{\eta=\xi(t)} = -1 \\ u(-\infty, t) = 0, & u(+\infty, t) = u_\infty, \\ u(x, 0) = u_0(x), & \eta \in \mathbf{R}, \end{cases} \quad (1)$$

Travelling waves are solutions such that ξ is linear, say $\xi(t) = \xi_0 - ct$, and u is of the form $u(t, \eta) = U_0(\eta + ct)$. After several transformations, we reduce problem (1) to an evolution equation in a suitable Banach space, in such a way that orbital stability/instability of the TW solution is equivalent to stability/instability of the null solution of the abstract equation. Due to the interface conditions, the final equation is fully nonlinear, i.e. of the form

$$\begin{cases} u'(t) = Lu(t) + F(u(t)), & t \geq 0 \\ u(0) = u_0, \end{cases} \quad (2)$$

where L is a linear operator in a Banach space X , and the nonlinear smooth perturbation F is defined on the domain $D(L)$ of L (more precisely, on a neighborhood of 0 in $D(L)$) and has values in X . Geometric theory of equations such as (2) includes results of local existence, uniqueness, regularity, stability, Hopf bifurcation. In particular, the principle of linearized stability holds, so that the problem of determining the stability of the TW solution of problem (1) is reduced to the problem of finding out the spectrum of L . In our case, L is nothing but the realization of a second order elliptic differential operator with suitable boundary conditions in the space X , and it is possible to characterize its spectrum. As a consequence, we are able to give a rigorous mathematical justification to previous formal computations.

Critical Conditions for Detonation Initiation
by Nonuniform Hot Pockets of Reactive Gases

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A numerical study of the critical conditions for detonation initiations in a cold reactive gaseous mixture is presented for one dimensional geometry. This study concerns initiation by a hot reactive pocket with nonuniform initial temperature. The Zeldovich criterion (1980) for the initiation of detonation at high temperature is found to be well verified. For a given initial temperature gradient, a CJ detonation is spontaneously developed at the temperature predicted by this criterion which is typically about 1100 K for a characteristic length scale of few centimeters. But a new phenomenon is exhibited: the same initial temperature gradient yields a quenching of the detonation at a lower critical temperature. Thus, the Zeldovich criterion is shown to not be sufficient to determine the critical conditions for detonation initiation in cold mixtures. These critical conditions are determined here in the planar geometry for an initial pocket (slab) of hot reactive mixture with a linear gradient of initial temperature embedded in a cold uniform mixture. For ordinary reactive mixtures, the typical critical size of such initial pockets to initiate detonation in cold gases at room temperature is of the order of 5 cm. For a smaller size the detonation is quenched before having reached the room temperature and the detonation initiation occurs only for larger sizes. An explanation of this quenching mechanism is provided as well as an analytical expression of the initiation criterion.

Numerical Simulation in Combustion:
Industry Needs and Perspectives

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Even if combustion is a very important subject for gas turbine manufacturers, this topic is often still approached quite empirically and the use of numerical codes is relatively limited.

Nevertheless, a wider utilization of computer simulations would be very effective in improving the design process, allowing to shorten the testing phase, to evaluate a larger number of alternative design options and, eventually, to save time and money.

The present industrial approach to combustion problems, with particular reference to FIAT Avio experience, is described and manufacturers' needs are highlighted, in order to give a guide-line for future cooperation between researchers and industries.

This cooperation should results in a mutual benefit, providing a fecund exchange of data and experiences. Tests on technological rigs and data coming from engine operations may be a very useful tool to check and improve the numerical models while, on the other hand, reliable models would give a dramatic enhancement of design activities, as already happened in other fields, like, for example, stress analysis or aerodynamics.

Combustion Stability of Solid Propellants

ZN- and FM- Approaches

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Theoretical investigations of nonsteady burning of solid propellants are based mainly on the approximation which takes into account thermal relaxation of the solid phase only. Within this approximation, there are two approaches to analysis named as Zeldovich-Novozhilov (ZN) and the Flame Modeling (FM) approaches. The main aim of this report is to point out at the equivalency of the two methods. As an example, the problem of combustion stability is taken. The well-known flame models such as Denison-Baum (DB) and Krier-T'ien-Sirignano-Summerfield (KTSS) models are discussed and compared with ZN-approach. It is shown that the stability condition are determined by only two parameters, which characterize the dependencies of burning rate and surface temperature on initial temperature in a steady-state regime.

Stability and Transient Radiation-Driven Solid Propellant Combustion

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Stability of radiation-driven steady-state combustion has been studied by the method of small perturbations. Stability boundaries are determined depending on the value of radiant flux and propellant transparency. The stability domain is found to become wider with increasing transparency and radiant flux.

Linear analysis of a burnrate response to harmonically oscillating radial flux predicts a decrease of resonance frequency when propellant transparency and radiant flux increase. For a resonance-type burnrate response, the maximum phase shift is realized at a frequency less than the resonance one. At low frequencies, the phase shift value is positive (shift advance) for semitransparent propellants and negative for highly transparent ones. At resonance, the phase shift is negative with absolute value being less than $\pi/2$. Numerical calculations revealed a good agreement with the results of linear analysis.

Nonlinear oscillating burnrate behavior is studied numerically. It is shown that, due to asymmetric form of the burnrate response, there is a misfit of phase shift determined in extrema (max, min) of the burnrate. The effect vanishes with increasing propellant transparency.

Transient burnrate behavior in the case of stepwise radiant flux action depends on propellant transparency and closeness of a burning regime to the linear stability boundary. If the final state (self-sustaining combustion) is close to the boundary of stability, the burnrate behavior after radiant flux cut off is characterized by an elongated transition for transparent propellant and extinction for semitransparent one. The reason is the nonconformity between the enthalpy excess in radiation driven combustion wave and that in steady-state self-sustaining combustion wave.

Acoustic Instabilities of Flames

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The excitation of acoustic vibrations by heat is related to a general phenomenon: the thermoacoustic instability which was first pointed out by Rijke in the middle of the XIXth century. Because of gas expansion, heat release in a gas flow acts as a volume source which may easily excite acoustic vibrations of the cavity. Lord Rayleigh gave a general criterion for a spontaneous amplification of acoustic modes by any local heat source: the local-energy addition or subtraction must be positively correlated with the pressure fluctuations. But this does not tell us when and how such a phenomenon may be produced in combustion and what are the basic mechanisms responsible for this coherence. Different examples are presented in this talk. Recent results of analytical studies concerning planar flames and cellular flames in premixed gas will be first recalled. Two other analytical results will be presented. A first one describes a new response mechanism of combustion of homogeneous solid propellants. It concerns the high frequency range where the non steady effects of the gas phase become dominant. A last one concerns the case of flames propagating in sprays or particle-laden gases where inertia and drag of particles may lead to a strong acoustic combustion instability. These analytical results have been obtained in the framework of the asymptotic analysis of non steady flame structures in the singular limit of an infinitely large reduced activation energy. Comparison with existing experimental data will also be presented.

Studies on Mathematical Models of Solid Propellant Combustion at NPU

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Three aspects of studies on mathematical models of solid propellant combustion conducted at Northwestern Polytechnical University (NPU) are reviewed in this paper.

First, based on SEM examination and X-ray photoelectron spectroscopy (XPS) test on quenched surface of AP-PU solid propellant, a mathematical model of propellant combustion is developed. The model considers the effect of molten binder covering the AP crystal surface, condensed phase reaction, and opposed gasification of AP covered with molten binder. In the model, the burning surface of solid propellant are divided into two regions. In region I, the AP crystal surface is covered with molten binder, and the opposed gasification of AP is proposed to take place under the covering binder layer. In region II, the BDP model well known is used. The two regions are connected with the same final adiabatic flame temperature. The ratio of area of region I to that of region II and its variation with pressure increasing are determined experimentally with XPS test. The model not only can be used to explain the plateau, mesa and normal burning features, but also can be used to analyze the effects of initial temperature and AP particle size on burning behaviors of composite solid propellants. Moreover, the model should be capable of providing a basis for studying the erosive burning and unsteady combustion of composite solid propellant, including those with negative pressure exponents.

Second, a simplified theoretical model is developed to consider the effect of thermal radiative heat transfer of combustion products on the combustion of aluminized propellants. From the model, a semiempirical method is deduced to predict the correlation of propellant burning rates in a combustion bomb, a subscale motor and a fullscale motor. The method possesses the advantage of being simple in calculation and of requiring less experiments.

The third is about the theoretical model of liquid quench of solid rocket motor. In the model, the coupling effects of motor ballistics, transient burning of solid propellants, liquid drop evaporation and heat transfer during cooling by liquid jet impinged on the burning surface are considered in detail. The spacewise thick flame model is used to describe the transient burning behavior of solid propellants. With the application of the model, the liquid quench process of solid rocket motor is predicted theoretically. The predicted critical injection pressure drop of liquid jet and liquid quantity required for reliable extinction are in good agreement with those measured experimentally.

In addition to the aspects above, the theoretical studies on ignition and erosive burning of solid propellants are also ongoing projects at NPU.

**Mathematical Modeling of Unsteady Combustion
of Energetic Solids Subject to External Radiation**

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A theoretical investigation is being conducted on the unsteady combustion of energetic materials and solid propellants under dynamic radiant heating conditions. The analysis has been carried out under the assumptions of quasi-steady gas and surface reaction, homogeneous propellant, and one-dimensional flame (or QSHOD theory; " t_c approximation" in Russian literature). The classical linear QSHOD theory has been generalized to include the effect of external radiant flux with in-depth absorption. This has been done in both the framework of the Zeldovich-Novozhilov (ZN) phenomenological theory and the flame modeling (FM) approach. The relationship of these two approaches has been demonstrated for the generalized radiant flux case. The nonlinear QSHOD theory has also been extended to include external radiation with in-depth absorption and some numerical studies of nonlinear effects have been conducted. These studies have illustrated an effect of the mean radiant flux on the combustion response (both linear and nonlinear) which has previously been neglected by most researchers in this area. The theoretical results have also illustrated the importance of in-depth absorption for most wavelength-material combinations. The effect of external radiation, including in-depth absorption, on the intrinsic stability of steady deflagration has also been investigated. It has been shown that, similar to the case with surface absorption, external radiation with in-depth absorption may have either a stabilizing or de-stabilizing effect, depending on how the temperature sensitivity varies with temperature. The principle of equivalence of external radiation and initial temperature has also been re-examined. Finally, analysis is extended to include effects such as distributed reaction in the condensed phase and a fully unsteady gas phase; some preliminary results are presented.

RADIATION-DRIVEN FREQUENCY RESPONSE FUNCTION BY FLAME MODELS

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Frequency response functions of solid rocket propellants, burning under sinusoidal fluctuations of pressure or external radiant flux, are discussed in the framework of linear perturbations. The γ flame model developed by this research group for spacewise thick flames is taken as reference for obtaining the needed perturbed boundary condition at the burning surface from the gas-phase side. All gas-phase developments are expressed in terms of the characteristic gas-phase time parameter proposed by MTS modelers in 1969. This formulation allows to recover as special cases all the results so far available in the competent technical literature and, in addition, is a good starting point for future developments permitting the effects of temperature on the gas-phase processes to be taken into account. Moreover, this unifying treatment is immediately derivable from the corresponding nonlinear analysis being carried out by this research group.

The alternative ZN (Zeldovich-Novozhilov) method, mainly developed in Russia, is quickly touched upon and compared to the FM (Flame Modeling) method pursued in this instance. Under proper assumptions, the two methods yield rather close results. Yet, considering the basic difficulties still facing modelers in this technical arena, it is suggested that both methods should be developed, hand-in-hand, in order to synergistically learn from both.

The effects of average radiant flux intensity and arbitrary surface layer absorption, previously neglected by this research group, are included and compared with results recently published in the open literature. The effects of pressure and several other operating parameters are examined as well. Among physical properties, the heat release at the burning surface and activation energy of the surface pyrolysis are most influential. The intrinsic combustion stability limits for linear burning are deduced and compared with some nonlinear expectations. Finally, the problem of sharp flames and relevance of pressure dependent surface pyrolysis is discussed.

Present developments are focused on the influence of gas-phase temperature on fluctuating heat feedback for both linear and nonlinear frequency response functions.

Derivation of Simplified Models in Chemical Kinetics

by

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When massively complex chemical kinetics problems are numerically investigated, the conventional methods of deriving simplified models are no longer viable. In general, these methods consist of two steps. First, the intermediates and fast elementary reactions must be identified. Then, the steady-state and partial-equilibrium assumptions must be applied to the intermediates and fast elementary reactions, respectively.

This process has many shortcomings. First of all, the difficulty in identifying the intermediates and fast reactions is proportional to the size of the full mechanism. Furthermore, the success of the conventional analysis requires a large amount of computations and relies heavily on the intuition and experience of the investigator. Finally, the results of such an analysis, depend on the assumptions made for the initial and operating conditions.

The Computational Singular Perturbation (CSP) method is a general method for the treatment of nonlinear ODE's which exhibit a boundary-layer type of stiffness. As a result, the method is very useful in the analysis of chemical kinetics problems. CSP identifies the fast reactions and intermediates and derives the appropriate relations among the elementary reaction rates, i.e. the steady-state and partial-equilibrium approximations. Since CSP is a computational method, the size and complexity of the kinetics mechanism as well as the dependence of the results to the initial and operating conditions pose no limitations on the successful use of the method.

The relations among different elementary reaction rates impose some constraints on the evolution of temperature and the species mass fraction. What really controls the system's evolution within these constraints is not clear. To answer this question, the original system of differential equations modelling the physical process must be simplified by the appropriate use of the relations among different elementary reaction rates. As it will be shown later on, this is an enormous task for an investigator, especially if the kinetics mechanism is large.

CSP can numerically perform this task requiring no outside input of any kind. The ability of CSP to properly identify the elementary reaction rates which locally control the evolution of temperature and species mass fractions and to simplify the system of differential equations provides important informations in the analysis of chemical kinetics mechanisms. First, the minimum set of unknowns can be selected so that no effort is wasted in monitoring unimportant to the investigator dependent parameters. In addition, the proper kinetics constants can be adjusted so that the numerical model provides a good representation of the experimental data.

The power of the CSP method in acquiring all the appropriate physical insights and in simplifying a large kinetics mechanism will be demonstrated for the case of homogeneous methanol oxidation at constant pressure.

International Workshop_
on
MATHEMATICAL METHODS IN COMBUSTION

List of participants

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